Supercritical water oxidation at microscale for space applications: A preliminary study

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1. Introduction

Several methods have been proposed in the literature to deal with the problem of organic waste and wastewater in space. Among these, supercritical water oxidation (SCWO) has been identified as one of the most promising candidate owing to its advantages over its competitors [1]. In addition to exhibiting characteristic properties of a supercritical fluid, such as high compressibility, supercritical water (SCW) behaves as a non-polar solvent in contrast to being polar at ambient conditions. Consequently, it acts as a very good solvent for organic matter and several non-polar gases, such as oxygen, nitrogen etc., which makes SCW a homogenous medium for the oxidation of organic matter. This forms the underlying principle of SCWO. The process occurs in a single phase overcoming the limitations posed by interfacial mass transfer facilitating fast reactions. Furthermore, no toxic products such as NOx, CO etc. are formed as temperatures are relatively low for their production, rendering SCWO a clean disposal method. Despite these advantages, the process is faced with two major challenges [1,2]. Firstly, corrosion of the process equipment due to reactive ions such as Cl^-, F^- and secondly, plugging of the reactors/process equipment due to the precipitation of potential inorganic salts. A simple strategy is to avoid reaching the temperature conditions which may lead to precipitation of salts. This is possible by injecting the feed (water + waste) at subcritical temperatures and attain supercritical conditions in the reactor by virtue of hydrothermal flames as an internal heat source [3]. Hydrothermal flames refer to the flames produced in the water due to combustion reaction between organic matter with oxidant in a SCW environment, primarily attributed to the reduction in the autoignition temperature of organic salts at high pressures.

While the literature is abundant in studies pertaining to SCWO using hydrothermal flames, these have been limited to ground-based applications and for meso-scale systems. In the current work, we aim to explore this process at microscale as a potential technology for the treatment of organic and human waste aboard ISS and future space missions [4,5]. The challenge lies to understand the behavior of flames confined within microreactor in zero-gravity and how it will govern the SCWO behavior when compared to ground conditions. As a first step, we highlight here the salient features for designing the microreactor and flame characteristics we can expect at microscale, for preliminary experiments using SCWO insert with DECLIC-evo.

2. Results

2.1 Design considerations for microreactor

One of the first step to realize the process at microscale is appropriate design of the microreactor. Excellent thermal and mechanical properties of sapphire in addition to its chemical compatibility with SCW renders it a suitable choice for realizing the reactor. A more significant design aspect is designing flow network and injector heads considering various factors. One of the initial constraints is to have a sufficient gap between the channels to minimize the risk of the reactor being ruptured by mechanical stresses following which the dimensions of the channel were set to be 300 µm for main channel with gap of 800 µm between them (Fig. 1). Secondly, designing the flow network and path is motivated by two primary objectives. (a) the oxidizer in the reactor will derived from the decomposition of H_2O_2 into H_2O and O_2 necessitating sufficient flow to ensure that enough time is available for decomposition of H_2O_2. (b) as the reactor is uniformly heated, it is desired that both the fuel and oxidizer stream enter the main channel at the same temperature. With oxidizer flow path constrained

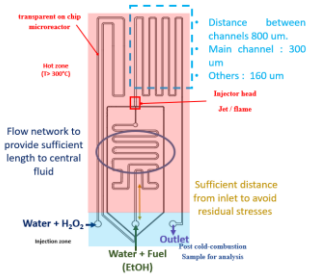

Figure 1: Schematic of the reactor

as explained in (a), the fuel flow path is desired to be of sufficient length to have enough residence time to attain the desired temperature. This was taken care of by providing a serpentine like flow path for the fuel stream. Final and the most important being the design of injector head, i.e., region of the main channel where the fuel and oxidizer are injected. In the current framework, we expect to have a non-premixed flame configuration where the combustion is primarily governed by mixing dynamics. Further, owing to the operation being in laminar regime, inefficient mixing may also lead to higher ignition lag and thus flame formation downstream in the main channel. However, space constraint at microscale calls for designs to reduce this delay and further provide means to anchor the flame near the entrance itself. In lieu of this, we propose designs wherein secondary flows have been created to cause certain degree of premixing before the fuel and oxidizer before entering the main channel. In addition, an island structure in the main channel is sought to provide a base to anchor the flame. Experimental result on Si-Pyrex system supports the premixing behavior and that injected H_2O_2 was decomposed into O_2 and H_2O (Fig. 2)

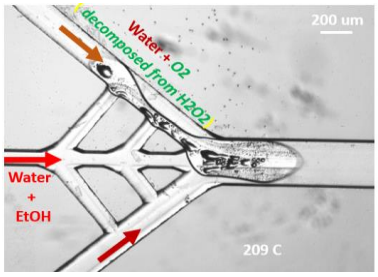

Figure 2: Observation of 2 phase flow due to decomposition of H_2O_2 to H_2O + O_2 (gas) at 110 bars.

2.2 DNS of hydrothermal flames

In order to optimize the reactor design and gain insights into the flame behavior, DNS studies are undertaken. We consider a single step irreversible reaction of oxidation of ethanol based on finite rate chemistry with rate kinetics being governed by Arrhenius law. We carry out simulations at initial pressure of 25 MPa and two different temperatures, 350 C and 400 C. These are primarily to draw out differences between subcritical and supercritical conditions of SCWO. Fig. 3 shows simulations for an injection flow velocity of 10 mm/s. An interesting feature is of sudden increase in flame temperature is observed owing to large amount of heat being constrained in such small volume. This highlights the need to cool the reactor to have steady flame as opposed to an intuitive thought to heat the reactor in order to ensure continuous operation with hydrothermal flames.

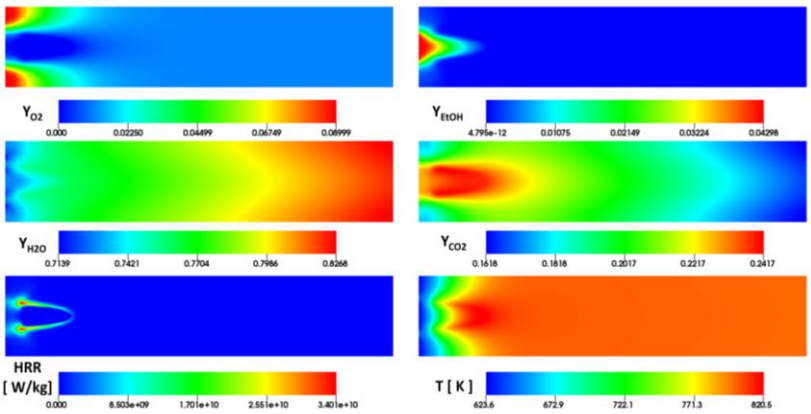

Figure 3: Contour plots for Tinjection = 350 C , U = 10 mm/s (both fuel and oxidizer) (Simulation done using NOTUS on supercomputer of CNES)

3. Perspective

The results obtained from simulations will be further investigated to seek insights into flame behavior as a function of different flow rates and fuel concentration. The objective is to figure out the flow window in which we can have a stable flame for a given concentration. These will be further verified via experiments in sapphire microreactor.

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